

CoreMS-AutoUpload: Automated Online Data Processing

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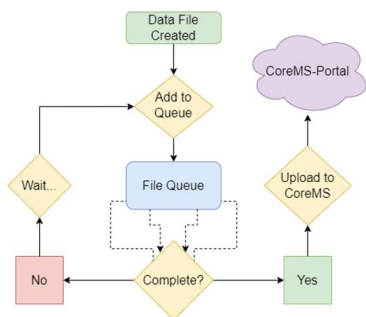
Introduction

CoreMS and CoreMS-Portal offers an easy means to process and visualize mass spectrometry datasets from a variety of instrument types. The main limitation in real-time data processing is the bottleneck resulting from the time required to manually upload data files.

As part of our ongoing work in lab automation, we have developed and deployed an instrument deployed software component to monitor and automatically upload/process acquired data, CoreMS-AutoUpload

Methods

1. A standalone software utility is downloaded from the CoreMS-Portal web interface.
2. The utility is executed and runs in the background on the instrument console and monitoring activated from the web interface.
3. Files matching an operator-defined pattern are automatically detected upon acquisition and uploaded to the CoreMS processing queue.
4. Results are available in the Portal immediately following processing for visualization.



AutoUpload Logic Flow

Discussion

The auto-uploader was initially developed as a component of a larger auto-calibration project, but the potential utility of the uploader on its own, allowing for data to be uploaded and processed without operator intervention, resulted in it being split out as a separate independent entity.

The AutoUpload package provides a straightforward and lightweight package, consisting of an executable file, (optional) setting configuration file and (optional) self-update utility. The AutoUpload executable itself needs no installation or special user privileges. All interaction is limited to the web portal and consists of starting/stopping monitoring and specifying the remote connection address:port. When operating, a simple console window is made available displaying status and any informational messages that may be generated.

AutoUpload: Key Features

1. Not directly tied to any vendor interfaces.
 - Currently tested with Thermo and Bruker data.
2. Built to target legacy instrument console hardware, requiring only => Windows 7.
 - Designed specifically for ease of porting.
3. Multiple file completion detection metrics implemented.
 - If the file format provides an "acquisition complete" flag, this is used. Otherwise, assorted file monitoring methods are used to determine if an acquisition is in progress and wait for completion.
4. Very light resource usage.
 - Even under artificial stress testing conditions, no significant load was observed on the host computer. (i.e., continuous ~3 s acquisitions)
5. Tolerant of poor network connections.
 - The uploader uses an internal queue to accumulate detected data events in case of network or other hardware issue. Upon connection reestablishment, queued files are processed in order of detection.

Pending Features

- Expansion to handle additional data formats.
- Improve visualization/web interface (In progress.)
- Adaptation to any new applications as user projects dictate.
- We are actively seeking ideas/directions from users!

Raw Data Auto-Uploader Allows New Automation Possibilities for MS Workflows



<https://github.com/EMSL-Computing/CoreMS-AutoUpload>